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## **DMol3/COSMO-RS Prediction of Aqueous Solubility and Reactivity of Selected Azo Dyes: Effect of Global Orbital Cut-off and COSMO Segment Variation**

*Tuesday, 5 December 2017 12:00 (20 minutes)*

### **HPC content**

I made use of the CHPC to get access to the Material Studio license and I also ran all my simulations on the CHPC cluster.

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